Victor S. Batista
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Biography

Victor S. Batista was brought up in Buenos Aires, Argentina, and received his *Licenciado en Ciencias Quimicas* (B. Sc. in Chemistry) degree from the *Facultad de Ciencias Exactas y Naturales (FCEyN) de la Universidad de Buenos Aires* in 1989. In 1991 he moved to the USA and received his PhD degree in Chemistry from Boston University in 1996, where he also received the Sugata Ray Award in 1995 working under the mentorship of Prof. David F. Coker on the development of theoretical and computational methods to investigate photochemical reaction dynamics in the condensed phase. Following two postodoctoral research programs, working on semiclassical methods with Prof. William H. Miller at the University of California, Berkeley (1997–1999) and coherent-control techniques with Prof. Paul Brumer at the University of Toronto (2000-2001), he joined the Yale faculty as an Assistant Professor of Chemistry in 2001, where he became Associate Professor of Chemistry in 2005, Full Professor with tenure in 2008 and John Randolph Huffman Professor of Chemistry 2019-22. He was Director of Undergraduate Studies (2008-2010). Since 2022, he is the John Gamble Kirkwood Professor of Chemistry at Yale University.

Batista has received the Innovation Award from Research Corporation (2002), the Hellman Family Junior Faculty Award from Yale University (2002); the Petroleum Research Funds Award G6 from the American Chemical Society (2002); the Career Award from the National Science Foundation (NSF) (2004); the Nanoscale Exploratory Research Award from NSF (2004); the Camille Dreyfus Teacher-Scholar Award (2005); an Alfred P. the Sloan Fellowship (2005–2006); co-chairmanship of the 2016 Vibrational Spectroscopy Gordon Conference; the 2016 Baker Lectureship at Cornell University; and the 2018 Harrison-MacRae Lectureship at Queen's University. He has been a Visiting Scholar of Phi Beta Kappa for 2017-2018. He has been awarded a 2022 Fulbright Fellowship. He has been a Fulbright Specialist since 2022. He has also been a Faculty Visiting Fellow at the Istituto Di Studi Superiori, Universita de Bologna. He is a member of the American Chemical Society (ACS PHYS Councillor 2018-Present), American Physical Society, and Biophysical Society.

He has published more than 430 articles in peer reviewed scientific journals (h=73) including the development and application of semiclassical and quantum dynamics methods for studies of photoinduced reaction dynamics, quantum control of excited state dynamics and mechanistic studies of photo- and electro-catalytic processes. He has developed quantum mechanics/molecular mechanics methods and applications to studies of catalytic processes in natural and artificial photosynthetic systems, including water-splitting in photosystem II and heterogenized catalysts on semiconductor and metallic surfaces. He developed methods for simulations of nonlinear optical spectroscopy (SFG) and inverse design methods for design of photosensitizers, rectifiers and catalysts for CO_2 reduction and H_2 evolution. He published studies of graph theory for the analysis of allosteric mechanisms in visual photoreceptors, olfactory receptors and catalytic enzymatic complexes, including CRISPR-Cas9 and IGPS.

Professional Preparation

Universidad de Buenos Aires (UBA): B.Sc. in Chemistry, 1989
Boston University: Theoretical Chemistry Ph.D. 1997
University of California, Berkeley: Theoretical Chem. Post-Doc. 1999
University of Toronto: Theoretical Chem. Post-Doc 2001

Appointments

July 2022-present: John Gamble Kirkwood Professor of Chemistry, Yale University.
July 2019-2022: John Randolph Huffman Professor of Chemistry, Yale University.
April 2020-present: Associate Editor, Journal of Chemical Theory and Computation.
April 2011-2020: Senior Editor, Journal of Physical Chemistry.
July 2008-July 2010: Director of Undergraduate Studies, Yale University
July 2008-present: Full Professor, Department of Chemistry, Yale University
July 2005-2008: Associate Professor, Department of Chemistry, Yale University.
March 2001-July 2005: Assistant Professor, Department of Chemistry, Yale University.

Selected Honors, Awards and Professional Service

2002 ACS PRF-G6 Award
2002 Hellman Family Junior Faculty Award
2002 Research Corporation Innovation Award
2004 NSF Career Award
2004 NSF Nanoscale Exploratory Research Award
2005-2006 Alfred P. Sloan Fellow
2005 Camille Dreyfus Teacher-Scholar Award
2005-2006 Yale Junior Faculty Fellow in the Natural Sciences
2016 Co-Chair of the Vibrational Spectroscopy Gordon Conference
2016 Baker Lecture, Cornell Univeristy
2017-2018 Phi Beta Kappa Visiting Scholar
2018 Harrison-MacRae Lecture, Queen's University
2018- ACS PHYS Councillor
2019-20 Visiting Fellow, Istituto Di Studi Superiori, - Universita de Bologna
2019- Member EU Academy of Sciences
2022 Fulbright U.S. Scholar Fellowship
Member: American Chemical Society, Biophysical Society

Synergistic Activities

Referee of scientific journals: Nature, Science, Proteins, Annual Review of Physical Chemistry, Proceedings of the National Academy of Science (U.S.A), Biophysical Journal, Journal of Chemical Physics, Chemical Physics Letters, Journal of Physical Chemistry, Journal of Inorganic Biochemistry, Journal of Chemical Theory and Computation, Journal of Computational and Theoretical Chemistry.

Panel reviewer committee member:

Review panels for NSF, DOE, NIH and ESF (ad hoc member of 25 panels to date). 2013-2017 NIH MSFA Permanent Member; 2015 NSF CCI Panelist; 2015 DOE PNNL Panelist; 2014-2013 DOE JCAP Review Panelist; 2013; DOE Career Program; 2013 NIH MSFE Study Section; 2013 NSF CHE Committee of Visitors; 2013 NSF CHE Theory Panel; 2012 NSF CCI Panel; 2012 NIH MSFE Study Section; 2012 DOE Career Panel;

DOE Theoretical Chemistry Review Panel, 2011; DOE BES Committee of Visitors, 2011; Chair, European Science Foundation Review Panel, EuroSolar Energy Program 2010; DOE Theoretical Chemistry Review Panel, 2009;NSF Review Panel Career Program, 2009; NSF Collaborative Research in Chemistry, 2005; Member, NSF Review Panel Career Program, 2005; Member, NSF Review Panel MRI in Chemistry, 2004.

Teacher mentor for the K-12 educational program e-mentoring initiative: Society for Advancement of Chicanos and Native Americans in Science (SACNAS).

Faculty service committees:
2020-2022 Physical Science & Engineering Area Committee & Tenure Appointments Committee (PSETAC); Theory Faculty Search Committee; Junior Faculty Mentoring Committees; Planning Committee

Teaching:
CHEM 584, Machine Learning and Quantum Computing in Chemistry
CHEM 472/572, Statistical Mechanics and Thermodynamics
CHEM 470/570, Introduction to Quantum Mechanics
CHEM 568, Advanced Quantum Mechanics
CHEM 505, Alternative Energy

Former Members of the Batista Group in Academic Positions:

1. Prof. Micheline Soley, University of Wisconsin-Madison, USA.
2. Prof. Jose Gascon, University of Connecticut, USA.
3. Prof. Luis G.C. Rego, Universidade Federal de Santa Catarina, Brazil.
4. Prof. Mehmet Ozbil Gebze, Technical University, Turkey.
5. Prof. Samuel Flores, Stockholm University, Sweden.
6. Prof. Robson da Silva Oliboni, Universidade Federal de Pelotas, Brazil.
7. Prof. Xin Chen, Xi'an Jiaotong University, China.
8. Prof. Ke Yang, Nankai Univerity, China
9. Prof. Junming Ho, University of South Wales, Australia.
10. Prof. Carlos Moyses Araujo, Karlstad University, Sweden.
11. Prof. Eduardo Sproviero, University of the Sciences, USA.
12. Prof. Atanu Acharya, University of Syracuse, USA.
13. Prof. Julio L. Palma, Pennsylvania State University, Fayette, USA.
14. Prof. Heidi Hendirckson, Lafayette College, USA.
15. Prof. Wendu Ding, Wake Forest University, USA.
16. Prof. Dequan Xiao, University of New Haven, USA.
17. Prof. Carmen Herrmann, Universität Hamburg, Germany.
18. Prof. Dr. Sandra Luber, SNSF Professor at University of Zurich, Switzerland.
19. Prof. Ivan Rivalta, Alma Mater Studiorum Universita Di Bologna, Italy.
20. Prof. Dalvin D. Mendez-Hernandez, Univ. of Puerto Rico-Cayey, Puerto Rico.

Graduate and Postdoctoral Advisors:

Ph.D. Advisor: **Prof. David Coker**, Boston University, Dept. of Chemistry
Postdoc Advisor: **Prof. William H. Miller** Univ. of California, Berkeley, Chemistry
Postdoc Advisor: **Prof. Paul Brumer**, Univ. of Toronto, Dept. of Chemistry

Graduate Students and Postdoctoral Associates
Total number of Ph.D. students supervised = 25
Total number of postdoctoral associates supervised = 34
Listed at http://ursula.chem.yale.edu/~batista/

Undergraduate research mentor: Underrepresented minority students enrolled in the STARS program at Yale University.

Developer of pedagogical web sites
http://ursula.chem.yale.edu/~batista/classes/CHEM584/index.html
http://ursula.chem.yale.edu/~batista/classes/vaa/index.html
http://ursula.chem.yale.edu/~batista/classes/v572/index.html
http://ursula.chem.yale.edu/~batista/classes/CHEM505/index.html
http://ursula.chem.yale.edu/~batista/classes/vvv/index.html
http://ursula.chem.yale.edu/~batista/classes/114/index.html
http://ursula.chem.yale.edu/~batista/classes/tutorials/index.html
http://wikidchem.org

Publications (total >340, *h*=73)
https://scholar.google.com/citations?user=0Df3zvEAAAAJ&hl=en

Selected Research Accomplishments

Time-Dependent Methods: The Batista group has developed time-dependent methods for simulations of photoinduced quantum reaction dynamics in polyatomic systems, including algorithms based on time-sliced semiclassical and full quantum-mechanical propagators (*e.g.*, the MP/SOFT method based on coherent state expansions and the TT-SOFT method based on tensor train networks). Applications of these methods have been focused on ultrafast relaxation processes that produce broad and structureless absorption spectra of polyatomic systems, including nonadiabatic interconversion dynamics, excited state intramolecular proton transfer, and photoinduced isomerization processes in excited electronic states.

Thermal Correlation Functions: In addition to quantum dynamics studies based on propagation of multidimensional wavefunctions, the Batista group has generalized the time-dependent algorithms to evaluate thermal-equilibrium density matrices, thermal correlation functions, and finite-temperature time-dependent expectation values. The generalized methods exploit the analogy between the time-dependent Schrödinger equation and the Bloch equation and computes finite-temperature density matrices via imaginary-time propagation, avoiding the "sign problem" that usually defies the capabilities of real-time path-integral Monte Carlo. The Heisenberg time-evolution operators, involved in thermal correlation functions, are analogously computed by real-time propagation.

Electronic Relaxation in Sensitized Semiconductors: Computational studies of sensitized semiconductor surfaces by the Batista group focused on metal-oxide surfaces (e.g., TiO_2) functionalized with organic and inorganic molecules, including photosensitizers and catalysts for photocatalytic cells. The studies characterized the nature of interfacial electron transfer mechanisms that for many years have challenged conventional electron transfer

theories formulated in the weak-coupling limit. The studies addressed the dynamics of photoinduced electron-hole pair relaxation at the molecular level, and the subsequent carrier diffusion mechanism after electron injection in the conduction band. In addition, coherent control scenarios based on sequences of ultrafast unitary laser pulses were computationally demonstrated, predicting the feasibility of creating and manipulating coherent electronic excitations on monolayers of adsorbate molecules covalently attached to TiO_2 semiconductor surfaces.

Photoanodes: Computational studies of TiO_2 surfaces sensitized with oxomanganese or Ir complexes by the Batista group have been focused on structure/function characterization with emphasis on catalytic mechanisms. The simulations suggested the possibility of visible-light photoactivation of catalysts attached to semiconductor surfaces, initiating a fruitful collaboration with 3 experimental groups at Yale (including Brudvig, Crabtree and Schmuttenmaer) in a joint experimental and theoretical effort to investigate TiO_2 functionalization for solar-light water-splitting and other applications of green-oxidation chemistry in the absence of primary oxidants.

Water Splitting in Photosystem II: The DFT-QM/MM studies of photosystem II (PSII) by Batista and coworkers addressed the development of chemically sensible models of the oxygen-evolving complex (OEC) in the $S_0 \rightarrow S_4$ states. The OEC of PSII is a paradigm system for engineering direct solar fuel production systems since it involves a catalyst with inexpensive and abundant metals (calcium and manganese) and is capable of splitting water by accumulating sufficient oxidizing power. The resulting scientific insight on structure/function relations provided by these computational studies of PSII has been useful not only to understand fundamental chemistry of oxygen evolution by natural photosynthesis, but also for studies of water splitting by artificial photosynthetic systems, including TiO_2 sacrificial electron-acceptor surfaces functionalized with oxomanganese catalysts.

Studies of Visual Rhodopsin: Computational studies of visual rhodopsin by Batista and coworkers have addressed the molecular rearrangements induced by the primary photochemical event responsible for phototransduction and energy storage. These studies provided fundamental insights on long-standing problems regarding the assembly and function of the individual amino acid residues and bound water molecules at the active site of this prototypical G-protein coupled receptor (GPCR) that is responsible for triggering the signal transmission cascade in vertebrate vision.

Coherent Control: The Batista group has developed quantum control scenarios for laser manipulation of electronic excitations in sensitized semiconductor surfaces. Building on earlier work on coherent-control of reaction dynamics in excited electronic states, it was found that superexchange hole tunneling through adsorbate molecules can be inhibited and eventually halted by applying sufficiently frequent unitary pulses that exchange energy with the system but do not collapse the coherent evolution, or affect the underlying electron transfer energy barriers.

Past and Upcoming Presentations (last 5 years >314 total)

Listed at http://ursula.chem.yale.edu/~batista/